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CFD Flow and Heat Transfer Simulation for Empty and Packed Fixed Bed Reactor in Catalytic Cracking of Naphtha

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***Abstract*—**This work aims to test the application of computational fluid dynamics (CFD) modeling to fixed bed catalytic cracking reactors. Studies of CFD with a fixed bed design commonly use a regular packing with N=2 to define bed geometry. CFD allows us to obtain a more accurate view of the fluid flow and heat transfer mechanisms present in fixed bed equipment. Naphtha was used as feedstock and the reactor length was 80cm. It is divided in three sections that catalyst bed packed in the middle section of the reactor. The reaction scheme was involved one primary reaction and 24 secondary reactions. Because of high CPU times in these simulations, parallel processing have been used. In this study the coke formation process in fixed bed and empty tube reactor was simulated and coke in these reactors are compared. In addition, the effect of steam ratio and feed flow rate on coke formation was investigated.

***Keywords*—**Coke Formation, CFD Simulation, Fixed Bed, Catalyitic Cracking.

I. Introduction

LIGHT olefins such as ethylene, propylene, and butanes are usually produced by the steam pyrolysis of naphtha or light alkanes. Two major limitations of the thermal process are the high process gas temperature (~1100K) required and the deposition of coke on the reactor walls which necessitates periodic shut-downs for decoking [1]. To overcome these limitations, several research efforts have focused on developing catalysts for pyrolysis, and the limited data available on catalytic pyrolysis has been summarized by Basu and Kunzru [2-3]. Most of the investigators have reported 12CaO-7Al2O3 to be the most active crystalline phase. A disadvantage of the 12CaO-7Al2O3 catalyst is the coke deposition on the catalyst. In recent years, there has been considerable interest in optimizing global efficiency in cracking processes and minimizing waste generation due to the general trend of market globalization, environmental actions, higher client expectations, and increased profit revenue for manufacturing companies. Computational fluid dynamics (CFD) is one of the critical "enabling technologies" for achieving this [4-6]. It allows process engineers to predict, manipulate, and design the desired fluid dynamics in process equipment. In the modeling and design of fixed bed equipment, CFD can be used to simulate single phase and multiphase flow through porous media and to perform detailed modeling of a packed bed cracking reactors, and it is used to design equipment with single-phase flow through a porous medium. It is known that the global behavior of a cracking process in a transport system depends directly on the local flow structure and heat transfer condition. There have been few CFD studies in fixed beds due to complex factors such as geometry definition and heat and mass transfer modeling, in addition to limitations in computational power. The first CFD approaches included 2D studies that resolved flow patterns and heat transfer without reaction insertion around proposed ideal geometries. [7-8]. In this paper 3D study of flow pattern in a fixed bed reactor is carried out. Coke formation in Naphtha catalytic pyrolysis is studied using CFD. Furthermore the heat transfer is studied in packed bed and empty tube.

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II. Geometry and Analysis

A. Geometrical Model

Geometrical modeling is one of the most critical stages in CFD simulation; correct definition of the geometry provides a more realistic scenario for the simulation, and the technique used for constructing the geometry will ensure the feasibility of generating a mesh good enough to capture all of the phenomena involved in the problem. The first step was to select a proper arrangement for the fixed bed. In a bed with a mixture of particle sizes if average particle size is used in the calculations, heat and mass dispersion follow the predictions for a bed of mono sized particles. [9] Due to complicated structure of catalyst bed it is assumed that catalyst granules have uniform spherical geometry with N=2 which N is the tube to particle ratio therefore, a homogeneous sphere stack was selected for this study. A Tow –layer arrangement (N=2, 58 spheres) with a 90° rotation around the reactor axis within each layer was chosen as the geometrical model for CFD simulations [10]. Fig. 2 and 3 show a lateral and isometric view of the constructed geometry, respectively. The mesh used in this study was the hybrid of tetra and hexagonal with the mesh interval of 0.3.

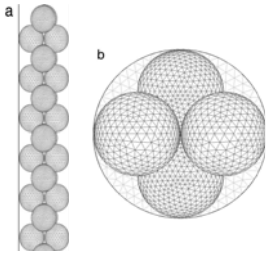


Fig. 1 CFD 58-sphere model used for validation purposes

B. Model Analysis

The fluid was taken to be incompressible, Newtonian, and in a laminar flow regime. Naphtha was chosen as the simulation fluid. Incompressible ideal gas law (for density) and first order upwind (for viscosity and species') were used in all simulations. The pressure-velocity coupling algorithm was the SIMPLE scheme.

C. Model Development

For modeling the experimental product yields, the large numbers of free radical reactions were approximated by a molecular model, consisting of a first-order primary reaction and 24 secondary reactions with coke formation reaction. The primary step represents the combined effect of the initiation, propagation, and termination reactions. It assumed that the coke precursors are aromatic compounds which are lumped (C_nH_{2n-6}). The kinetic parameters of coke formation were extracted from literature articles [2-3].The Navier-Stokes equations and energy balances were solved with kinetic equation of 27 reaction.

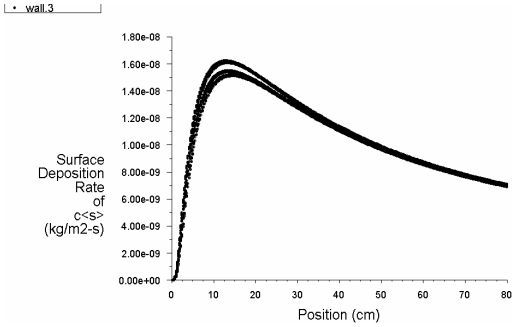
D. Parallel Processing

The primary goal parallel processing is to reduce calculation turnaround times by using multiple processors (CPUs). In this simulation each processor has its own (private) memory associated with it. The processors communicate with each other through a socket communicator, or MPI. Message-passing software is loaded on every computer in the cluster and a Windows process is started. Through the interface, computers coordinate their tasks, such as sending and receiving arrays, synchronizing, and performing global operations (such as summations over all cells), by sending and receiving messages to and from one another.

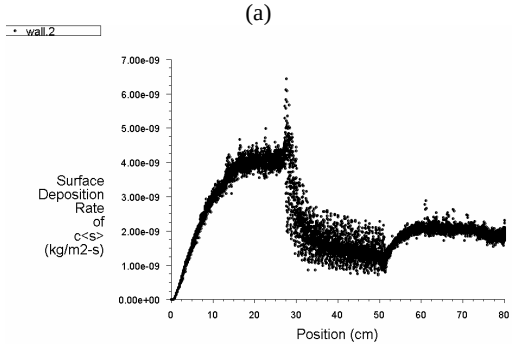
III. Results and Discussion

A. Effect of Flow Rate in Coke Formation

In Fig. 2 (a,b) the amount of coke deposition in empty tube and fixed bed reactor was compared respectively. As can be seen, the catalyst has significant effect on coke deposition on fixed bed reactor. In fixed bed reactor there is an increase in coke deposition in the initial part of catalyst bed.



(a)



(b)

Fig. 2 Coke deposition profiles in empty (a) and fixed bed reactor (b) (S.R=0.1, Flow rate=0.0002(kg/s))

As the reaction is progressing due to decreasing of coke precursor concentration, the coke deposition profile has decreasing trend. The effects of flow rate on coke deposition were investigated in Figs. 2, 3 and 4. It can be seen that increasing of flow rate has significant variation in coke profiles.

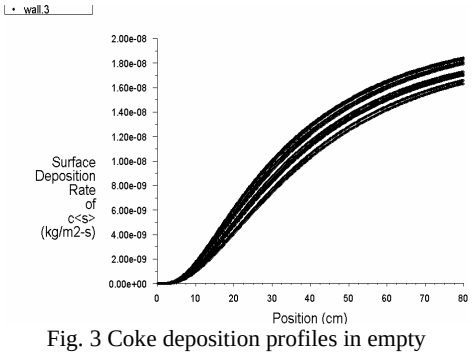


Fig. 3 Coke deposition profiles in empty

In these figures the thickness of graph indicates the coke deposited thickness in the reactor. As can be seen in the Fig. 4 the counters of coke deposition on catalyst bed are demonstrated which it is confirm the results that shown in Figs. 3 and 4. Fig. 6 indicates the coke deposition profiles in empty tube reactor in different steam ratios. As can be seen in Fig. 5 that the coke deposition decrease with increasing steam ratio due to low concentration of Naphtha in high steam ratios

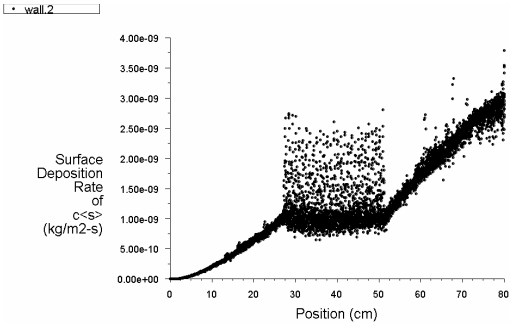
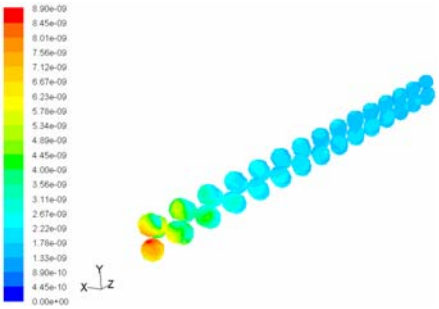


Fig. 4 Coke deposition profiles in fixed bed reactor (S.R=0.1, Flow rate=0.002(kg/s))



(a)

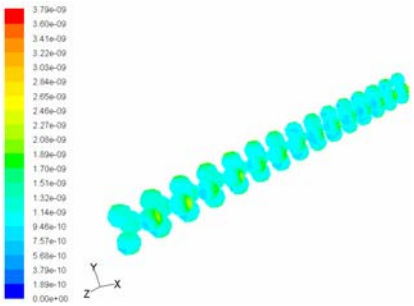


Fig. 5 Coke deposition profiles in fixed bed reactor in two flow rate 0.00002(kg/s) (a) and 0.0002(kg/s) (b)

B. Effect Steam Ratio

In Fig. 6 effect of steam ratio on coke deposition rate was investigated, in both empty and packed bed tubes, with increasing of steam ratio the Naphtha concentration is decreased and therefore there is a decline trend in coke deposition profiles. In empty tube there is a same effect of steam ratio on coke deposition on the wall of the reactor.

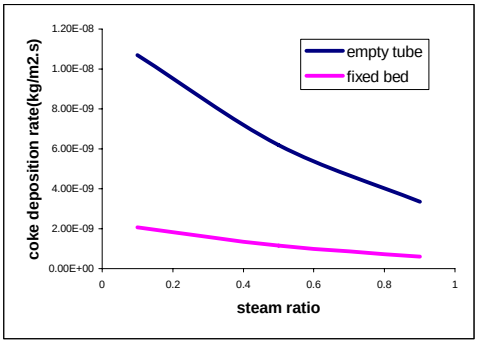


Fig. 6 Coke deposition in fixed bed and empty tube in different steam ratios

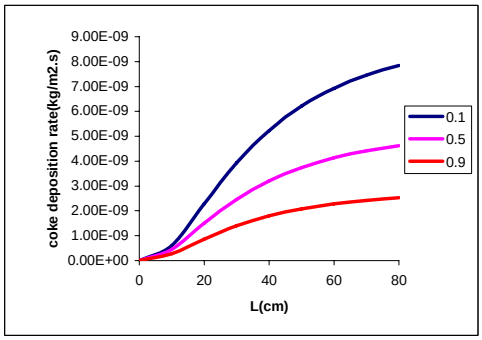


Fig. 6 Coke deposition in different steam ratio in the empty reactor tube

B. Effect of Vorticity and Stagnation Points on Coke Distribution

In Fig. 7 the coke deposition rate and the effect of vorticity was investigated. It was shown in the Fig. 7 the coke deposition rate in the stagnation points are more than the other places in the reactor. This caused more deposition of coke on the contact surface of catalysts with reactor wall and other catalyst granules. In addition to, because of secondary flows in the fixed bed, there is an increasing in residence time and therefore the coke deposition is increased.

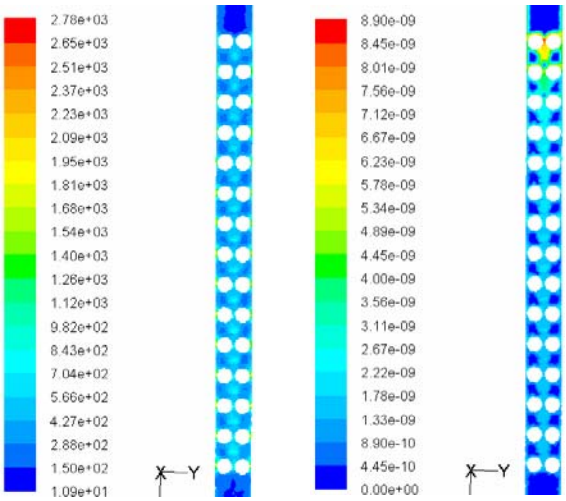


Fig. 8 Vorticity contours (left) and coke deposition rate contours (right) on x-coordinate surface in fixed bed reactor (S.R=0.1, Flow rate=0.00002 Kg/S)

C. Effect of Catalyst Bed on Heat Transfer

The wall Nu number of fixed bed and empty tube reactor was shown in Fig. 8. As can be seen the wall Nu number in both fixed bed and empty tube reactor is increased with feed flow rate. But Nu number in fixed bed reactor is more than empty tube reactor due to the vorticity and stagnation points in the catalyst bed. In addition because of less coke deposition in the fixed bed reactor the heat transferred with more quality.

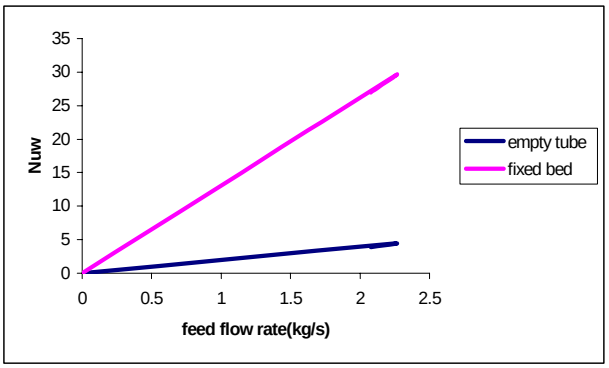


Fig. 8 Wall Nu number of fixed bed and empty tube reactor indifferent flow rate

IV. Conclusion

In this paper the coke deposition were studied with CFD in both fixed bed and empty tube reactor. It was found that:

1) The coke deposition profile is changed with variation of flow rate.
2) The coke deposition is decreased with increasing steam ratio in both fixed bed and empty tube reactor.
3) Stagnation points and vorticity are two important factors on coke deposition.
4) Because of more stagnation points in packed bed reactor, the Nuselt number is increased by increasing of inlet flow rate.

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